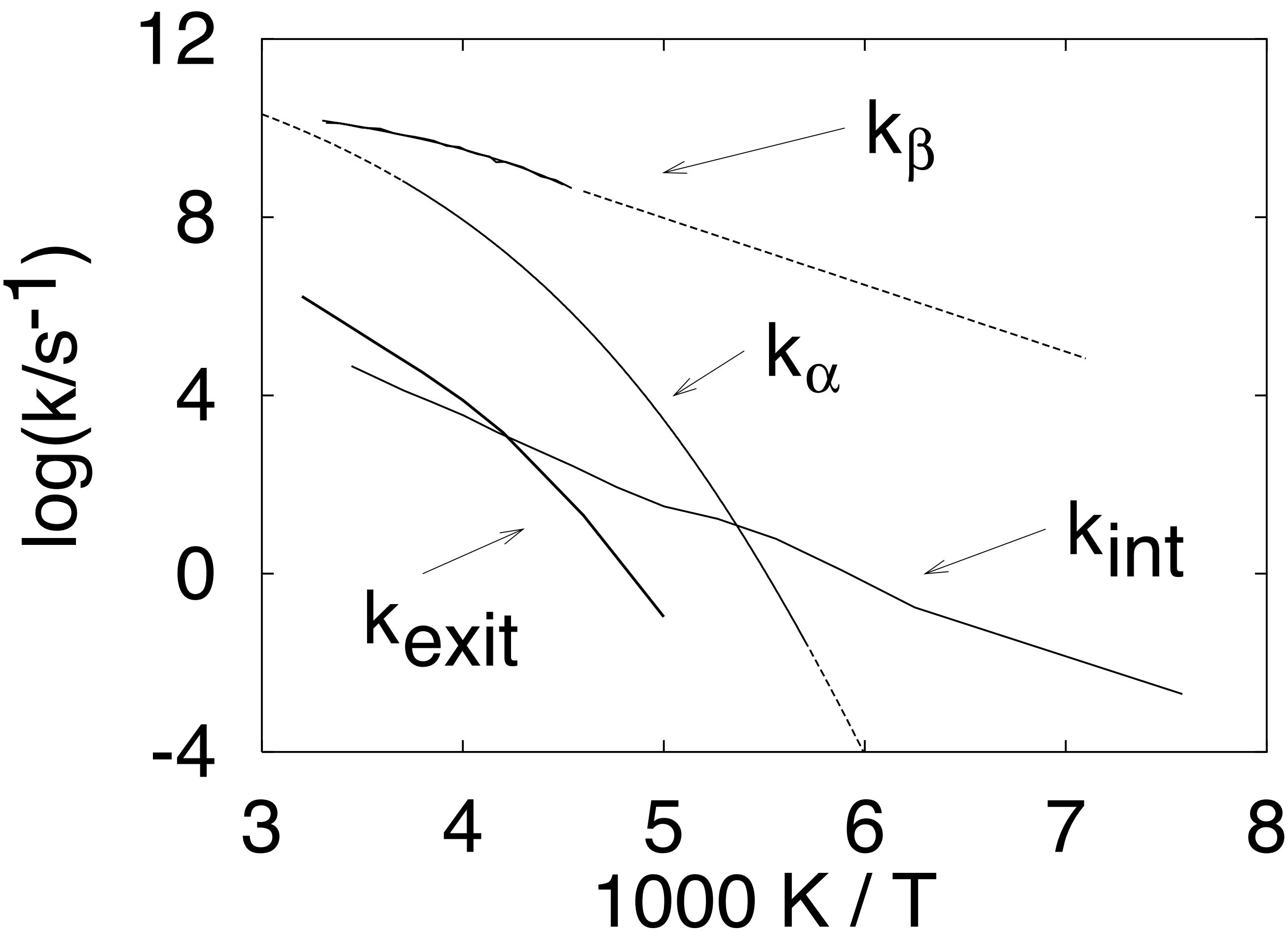
Organizational Summary



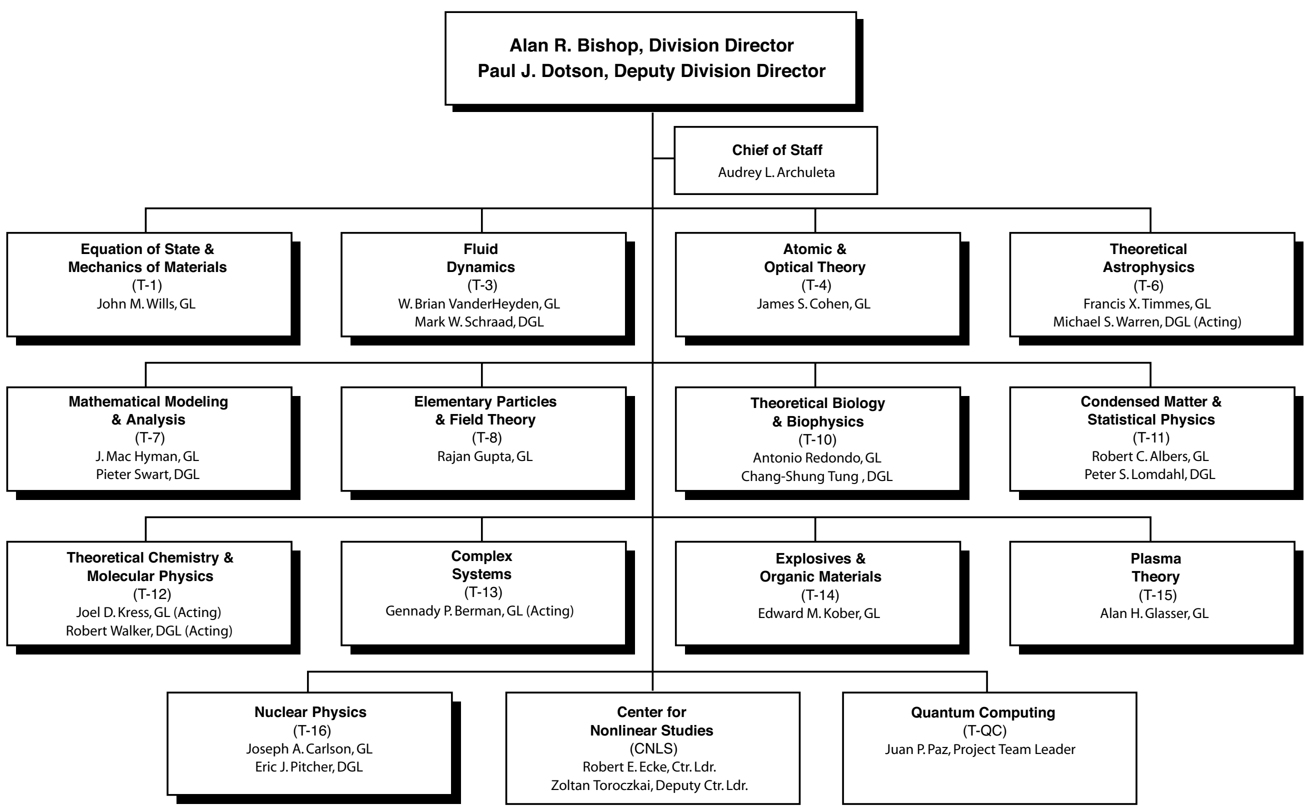
ORGANIZATIONAL SUMMARY

The mission of the Theoretical (T) Division is to perform theoretical research to further our scientific understanding of the physical world; to establish a technical foundation for current and future defense, civilian, and industrial needs; and to explore interdisciplinary frontiers of scientific endeavor.

In addition to participating in large Los Alamos National Laboratory projects, the Theoretical Division nurtures smaller projects for their intrinsic scientific and technical interest to the Laboratory and the Nation. A major role of the Theoretical Division is that of innovator and incubator for future technical directions of the Laboratory. Frequently these projects reach a level of development that attracts significant program funding and has, in the past, led to the establishment of new divisions.

The activities of the 13 groups, the Center for Nonlinear Studies, and the Special Projects Office span much of theoretical science. Because of the breadth of the Division's work, essential contributions are made to each of the Laboratory's core competencies and strategic goals as demonstrated by the activities of the groups.

THEORETICAL (T) DIVISION



Theoretical Division Office/Special Projects Office-Quantum Computing (T-DO)
Division technical staff are engaged in special projects that do not organizationally fit into an established group in the Division. A major effort is the study of the transition from quantum to classical ("decoherence") physics, and the study of quantum-based information and computing and their associated technology, closely coordinated with the Los Alamos Quantum Institute. In addition, technical staff members carry out research in relativistic heavy ions, high-spin states in nuclei, neutron physics, electronic and structural materials, and nonlinear science. **Technical staff includes: 7 Technical Staff Members (including 2 Senior Fellows and 4 Fellows), 2 Limited-term Technical Staff Members, 1 Postdoctoral Associate, and 2 Graduate Research Assistants.**

Equation of State and Mechanics of Materials (T-1)
T-1 develops theory and computational models to describe the Equation of State and Mechanics of Materials (EOS/MOM), including, but not limited to, materials of interest to nuclear weapons, and implements these models in computer codes that contribute in particular to the SESAME Equation-of-State and Materials Properties Library, which is maintained by T-1. The group has an active research program outside the EOS/MOM program developing theory, methodology, and calculation to support and enhance that program, funded by sources both internal (Laboratory Directed Research and Development) and external (Department of Defense, Advanced Fuel Cycle Initiative, and others) to the Laboratory. Relevant areas of research include strong electron correlation; actinide electronic structure; first-principles prediction of mechanical and thermodynamic properties of multicomponent materials; multiphase EOS theory; microscopic, mesoscopic, and continuum-level mechanical behavior of materials; Direct Numerical Simulation of materials properties; energetic materials; grain growth phenomena; and order-N numerical techniques for electronic structure calculation. Capability developed in support of EOS/MOM is used to support related programs such as Pu aging studies and other projects in the nuclear and conventional defense communities, civilian research communities, commercial applications, and threat reduction. **Technical staff includes: 13 Technical Staff Members (including 1 Fellow), 4 Limited-term Technical Staff Members, 4 Postdoctoral Associates, and 1 Graduate Research Assistant.**

Fluid Dynamics (T-3)
T-3 staff members are involved in modern hydrodynamic theory, materials modeling, and computational simulations. There is an emphasis on coupling advanced numerical methods for fluid dynamics at all flow velocities with models for other processes, including chemical reactions, phase change, heat and mass transfer, plasma behavior, constitutive properties of structural materials, and combustion. Advanced models and methods are incorporated in fully functional 2- and 3-D computer simulation codes and implemented on the full spectrum of computing hardware from high-performance workstations to massively parallel supercomputers. Current application areas include nuclear and conventional weapons, internal combustion engines, structural materials, process chemistry for the oil and gas industries, ferrous metals and chemical industries, models for casting, and circulation models for the global ocean. **Technical staff includes: 27 Technical Staff Members, 1 Limited-term Technical Staff Member, 2 Postdoctoral Associates, and 2 Graduate Research Assistants.**

Atomic and Optical Theory (T-4)
T-4 staff members develop methods for and perform calculations of atomic structure, scattering cross sections, opacities, exotic atoms, and quantum and nonlinear optics, including effects of high energy-density environments and interaction with external electromagnetic fields. Current efforts include the evaluation of opacities for a wide range of physical conditions, nonequilibrium kinetics, quantum molecular dynamics simulations of dense plasmas and shocked hydrocarbons, hohlraum spectroscopy, plasma sources of x-ray ultraviolet radiation, strong-field ionization and scattering, decoherence and chaos, quantum computing, and Bose-Einstein and Fermion condensates of cold atoms. The group provides interactive web sites for user calculations of opacities of mixtures and for calculations of atomic structure and cross sections. It also organizes and partially sponsors the annual Los Alamos Summer School for undergraduate students in physics. **Technical staff includes: 7 Technical Staff Members (including 1 Fellow), 4 Limited-term Technical Staff Members, and 8 Postdoctoral Associates.**

Theoretical Astrophysics (T-6)
T-6 staff members are involved in (1) studies of stellar evolution including supernovae, intermediate mass stars, nucleosynthesis, and oscillations; (2) nuclear physics and its applications; (3) large-scale structures in the universe; (4) relativistic astrophysics involving compact objects such as white dwarfs, neutron stars, and black holes; (5) comets and asteroids in the solar system; and (6) planetary interiors and evolution. The group has considerable strength in computer and computational science issues underlying multidimensional simulations and the analysis of massive data sets. T-6 is exceptional among theoretical astrophysics organizations across the Nation in its explicit emphasis on connecting fundamental science to national needs and Laboratory missions. **Technical staff includes: 8 Technical Staff Members (including 1 Fellow), 3 Limited-term Technical Staff Members, 5 Postdoctoral Associates, 3 Graduate Research Assistants, and 4 Undergraduate Students.**

Mathematical Modeling and Analysis (T-7)
T-7 combines the strengths of applied mathematicians, mathematical physicists, and numerical analysts to derive, analyze, and solve mathematical models of complex problems. Its mission is to conduct forefront basic and applied

research in mathematical modeling and analysis, provide theoretical leadership and support for the Laboratory and other programs of national interest, and to furnish an effective interface with academic science. In accordance with this mission, T-7 maintains its multidisciplinary, but highly mathematically oriented character, by supporting a strong applied research effort that is grounded in basic research. The applied mathematicians in T-7 have made substantial contributions in solving large systems of linear and nonlinear equations, in the theoretical and numerical solutions of nonlinear partial differential equations, in modeling the long-time predictability of ocean dynamics, in nonlinear optical transmission lines, in the applications of wavelets, in applied stochastic modeling and deriving effective parameters for homogenizing multiscale problems, and in the mathematical modeling of disease transmission and pattern formation in biological systems. **Technical staff includes: 8 Technical Staff Members, 11 Limited-term Technical Staff Members, 6 Postdoctoral Associates, 6 Graduate Research Assistants, and 1 Undergraduate Student.**

Elementary Particles and Field Theory (T-8)
T-8 conducts research in particle physics, both on the standard model of electromagnetic, weak and strong interactions, and on theories that extend it. This includes a strong program in computational quantum chromodynamics to calculate the hadron spectrum, quark masses, and weak matrix elements, especially those that are required to quantitatively understand the experimentally observed CP violation. There is a significant effort to elucidate the structure of theories that invoke supersymmetry and extra dimensions. Cosmology, particle-astrophysics, gravity, and large-scale structure of the universe are growing activities in the group. Fundamental issues of quantum field theory forms another key focus of research, especially in the arena of systems far from equilibrium and the study of long-distance structure of quantized gravity. Multidisciplinary efforts include studies at the interface of elementary particle physics, nuclear physics, and astrophysics; application of scaling ideas to biological and ecological systems; the study of viral evolution with an eye to understanding and controlling the AIDS epidemic; and studies of the formation and evolution of structure in the universe. Efforts in quantum science and technology include understanding the emergence of classical behavior from underlying quantum dynamics and designing feedback control for quantum dynamical systems. Computational science is a major thrust area, with applications to scaling theory to stochastic equations for nonequilibrium dynamics, modern dynamical systems theory for accelerator design, and the study of biological systems. This group maintains close ties with experimental efforts in neutrino physics and astrophysics, satellite tracking, cosmological surveys, and has made a major contribution to the production and trapping of anti-hydrogen. **Technical staff includes: 6 Technical Staff Members (including 1 Fellow), 1 Limited-term Technical Staff Member, 4 Postdoctoral Associates, 8 Graduate Research Assistants, and 1 Undergraduate Student.**

Theoretical Biology and Biophysics (T-10)
T-10 focuses on the modeling of biological systems, molecular modeling, and the analysis and informatics of molecular and cellular biological data. Its activities reflect the needs both to further our understanding of living systems at the cellular and molecular levels and to improve the Nation's health and economic welfare. T-10 is one of the few research groups in the world devoted to mathematical modeling and computational analysis of problems in cellular and molecular biology. T-10 has created and is responsible for the maintenance of the HIV, HCV (Hepatitis C virus), and Influenza Sequence Databases, as well as the HIV Immunology Database and the HIV Resistance Database. Research efforts span a number of topics including understanding dynamics and treatment of viral diseases such as HIV, influenza, and hepatitis; immune system modeling; receptor-ligand interactions and cell signaling; computational aspects of the human genome initiative; pattern recognition in DNA sequences; high-performance computational studies of macromolecular structure and dynamics; RNA structure; membranes and membrane proteins; protein function and dynamics; and protein folding. **Technical staff includes: 13 Technical Staff Members (including 2 Senior Fellows and 1 Fellow), 6 Limited-term Technical Staff Members, 7 Postdoctoral Associates, 8 Technicians, 3 Graduate Research Assistants, and 2 Undergraduate Students.**

Condensed Matter and Statistical Physics (T-11)
T-11 conducts research in condensed matter theory including electronic, structural, and transport properties of metals, semiconductors, compounds and alloys; microscopic modeling of materials properties and textures; fundamental studies of nonlinear and nonequilibrium systems; quantum field theory and algebraic approaches to statistical mechanics and materials physics; investigations of the properties of heavy fermions, high-temperature and organic superconductors and other strongly correlated electronic systems; phenomenology and other aspects of layered anisotropic superconductors; development of advanced algorithms for scientific computing (e.g., quantum Monte Carlo, molecular and Langevin dynamics involving multiple time and length scales) and the development of visualization tools for large data sets; magnetoresistance in perovskites; Ginzburg-Landau models of elastic, martensitic, and displacive phase-transformation

materials; microscopic aspects of shock waves in materials; aspects of quantum information related to condensed matter systems; device physics; nanophysics and nanotechnology; and applications of condensed matter physics to soft matter (polymers, organics, and biomaterials). **Technical staff includes: 11 Technical Staff Members (including 2 Fellows), 5 Limited-term Technical Staff Members, 9 Postdoctoral Associates, 3 Graduate Research Assistants, and 1 Undergraduate Student.**

Theoretical Chemistry and Molecular Physics (T-12)
This group is staffed by theoretical chemists and physicists who work on projects aimed towards an improved understanding of the behavior of matter. Generally, projects seek to describe how basic forces operating at the atomic, molecular, and mesoscopic level manifest themselves in the properties of matter at more macroscopic scales. Current activities include research both in gas-phase and condensed-phase phenomena and projects apply state-of-the-art computational approaches in fundamental and applied studies of the physics and chemistry of molecules and materials. Research projects include the development and application of techniques for calculating the electronic properties of molecules, the dynamics and kinetics of chemical reactions, atomistic simulations of materials, molecular modeling of catalysts, the study of solute-solvent interactions, and chemical and biological process modeling. **Technical staff includes: 13 Technical Staff Members (including 2 Fellows), 3 Limited-term Technical Staff Members, 9 Postdoctoral Associates, and 2 Graduate Research Assistants.**

Complex Systems (T-13)
T-13 creates new methods for solving complex problems and applies them to problems at the forefront of technology. This group also initiates and coordinates work on complex systems throughout the Division. Incomplete knowledge of the factors that govern the behavior of complex systems leads to the need for a probabilistic description. In keeping with this fact, T-13 has a strong program in several branches of statistical physics. This work includes complex networks, statistical fluid dynamics, with application to turbulent and multiphase fluid mixing, granular flow, and modeling of fluid flow in petroleum reservoirs. Each of these efforts has a theoretical and computational component, which is also closely tied to experiment. Another strong effort involves the modeling of laser-matter interactions for inertial confinement fusion studies. A vigorous program on uncertainty quantification addresses the problem of assigning error bars or confidence levels to predictions based on large-scale simulations. Computational and theoretical work on complex biological systems is represented by research on the spread of influenza, recognition mechanisms for protein-DNA binding, control of transcription, and regulation of gene expression. Modeling and simulation of nanodevices and large quantum computers is also an active area of research that has attracted wide interest. **Technical staff includes: 11 Technical Staff Members, 1 Long-term Visiting Staff Member, 2 Limited-term Technical Staff Members, and 6 Postdoctoral Associates.**

Explosives and Organic Materials (T-14)
The group is involved with the modeling and prediction of the properties and response characteristics of explosives and other organic materials, particularly polymers. A majority of the work is funded by the nuclear weapons program and has direct impact on both stockpile certification calculations and the design and analysis of experiments for validation purposes. Within that context, T-14 strives to obtain fundamental understanding of the various processes involved and connect them together with appropriate multiscale modeling programs. This group interacts strongly with other groups within the Division, Laboratory, and universities to accomplish this goal. Topics of general interest are the mechanical and reactive behavior of organic crystals and polymeric materials, ignition and detonation characteristics of explosive formulations, and how detonation and explosion waves interact with other materials. Included within the group is expertise in hydrodynamics and shock interactions, reactive flow simulations, equations of state for organic materials, molecular modeling with classical and quantum mechanical methods, micromechanical simulations, and material response characterization. Current projects include studies of the initiation and burn processes in damaged and intact explosive materials, advanced energetic equations of state, response characteristics of composite polymeric materials, and the prediction of materials and chemical reaction properties with molecular modeling. These efforts support advanced defense applications, including nuclear and counterterrorism programs. **Technical staff includes: 8 Technical Staff Members, 2 Limited-term Technical Staff Members, 3 Postdoctoral Associates, and 3 Graduate Research Assistants.**

Plasma Theory (T-15)
T-15 studies the theory of the fourth state of matter (after solid, liquid, and gas), plasma, or ionized gas. Most of the matter in the universe is in the plasma state: flames, fluorescent lights, the earth's magnetosphere, the sun, the stars, nebulae, thermonuclear explosions, plasmas confined in magnetic fields for magnetic fusion energy, and plasmas used for industrial processing. Because plasmas are ionized and carry electric currents, they interact strongly with electromagnetic

fields. This group studies the basic properties and collective motions of plasmas and electromagnetic fields. A major activity is development of efficient, parallel computer codes for the modeling and simulation of plasmas, using both fluid and kinetic descriptions. Numerical simulation of magnetized plasmas is particularly challenging because of the high degree of anisotropy and large range of length and time scales. Some codes developed by T-15 are in wide use throughout the U.S. magnetic fusion community, including the NIMROD toroidal simulation code, the DCON code for rapid determination of the stability of axisymmetric toroidal plasmas, and the CHIP code for modeling helicity injection into tokamaks. Other more powerful codes are under development using advanced numerical methods. Another topic of interest is astrophysical plasmas, particularly the behavior of plasmas undergoing magnetic reconnection, and their role in the evolution of active galactic nuclei. A relatively new and rapidly growing area of emphasis is the study of strongly coupled plasmas of interest in high energy-density physics. **Technical staff includes: 7 Technical Staff Members, 1 Limited-term Technical Staff Member, 4 Postdoctoral Associates, and 6 Graduate Research Assistants.**

Nuclear Physics (T-16)
T-16 staff members study nuclear reaction mechanisms, nuclear structure, and provide nuclear data to the Laboratory and Nation. Current efforts include the modeling of neutron and charged-particle cross-sections and spectra (including reactions on isomers and nuclides off the line of stability); improvement of fission theories and models of high-energy heavy ion reactions; developing sophisticated codes and libraries for transmutation and radioactivity calculations; high-energy scattering and cascade models; nuclear data processing and testing for use in radiation transport codes; performing exact calculations of few-body systems; the study of chiral symmetric perturbation theory; the production and decay of hypernuclei; structure of exotic nuclei and hadrons; and experimental implications of proposed new fundamental physical interactions and fundamental symmetries and violations thereof, with an emphasis on neutrino physics, CP-violation, and rare decays of mesons. Applications include nuclear weapons design, proton radiography, counterproliferation, astrophysics, advanced fission and fusion reactor analysis, radiation shielding, radiotherapy, accelerator-driven systems and power sources for space satellites. **Technical staff includes: 14 Technical Staff Members (including 2 Fellows), 4 Limited-term Technical Staff Members, and 5 Postdoctoral Associates.**

Center for Nonlinear Studies (CNLS)
CNLS identifies and studies fundamental nonlinear and complex problems and promotes the use of the results in applied research. It stimulates interdisciplinary research and information exchanges inside and outside the Laboratory and provides a Laboratory focal point for collaboration with academic and other centers of excellence in nonlinear science. CNLS disseminates recent developments in nonlinear science and introduces students and postdoctoral researchers to this subject. The Center achieves these goals by hosting and co-hosting conferences and workshops; through extensive visitor, postdoctoral, and student programs; and through interactions with Laboratory staff. The major research areas include networks research with applications to biology, information science and agent-based systems, biological physics, statistical physics and nonequilibrium statistical mechanics, turbulence, condensed matter physics (both soft materials and electronic properties), and computer science. **Technical staff includes: 2 Technical Staff Members (including 1 Fellow), 19 Postdoctoral Associates, and 2 Graduate Research Assistants.**